propan-2-yl naphthalen-1-ylacetate 68360-82-7 | DTXSID60286262

00300-02-7	D1731D00200202	

Model Performance

N.A. I. I.	D .
Model	II)ata
IVIOGCI	Data

Weighted KNN model

5-fold CV (7	75%)	Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 6.39e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.07e-01

Confidence level: 6.43e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl cinnamate

Measured: 1.00e-05 Predicted: 1.73e-02

Image not found

Clorophene

Measured: 2.24e-04 Predicted: 1.28e-05

Image not found

Butam

Measured: 1.19e-06 Predicted: 8.05e-04

Image not found

Benzoic anhydride Measured: 1.70e-03 Predicted: 6.04e-05